Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis{3-[4-(1*H*-imidazol-1-yl)-phenyl]-5-(pyridin-2-yl-κN)-1*H*-1,2,4-triazol-1-ido-κN^1}zinc

You-Song Wang, Guang-Mei Qiu and Cui-Juan Wang*

Department of Chemistry and Chemical Engineering, College of Life Science and Bioengineering, SouthWest JiaoTong University, Chengdu, Sichuan 610031, People's Republic of China
Correspondence e-mail: ejuan6046@sina.com

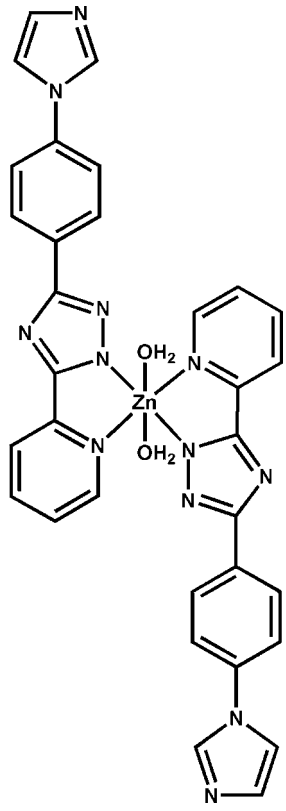
Received 22 June 2012; accepted 10 August 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.109; data-to-parameter ratio = 12.3.

The centrosymmetric molecule of the title compound, $[Zn(C_{16}H_{11}N_6)_2(H_2O)_2]$, contains one Zn^{2+} ion located on a center of symmetry, two 3-[4-(1*H*-imidazol-1-yl)phenyl]-5-(pyridin-2-yl)-1*H*-1,2,4-triazol-1-ide (Ippyt) ligands and two coordinating water molecules. The Zn^{II} ion is six-coordinated in a distorted octahedral coordination geometry by four N atoms from two Ippyt ligands and by two O atoms from two water molecules. Adjacent units are interconnected though O—H···N hydrogen bonds, forming a three-dimensional network.

Related literature

For similar structures, see: Braga *et al.* (2005); Lin *et al.* (2010); Faulmann *et al.* (1990); Han *et al.* (2005); Xue *et al.* (2009).



Experimental

Crystal data

$[Zn(C_{16}H_{11}N_6)_2(H_2O)_2]$
M_r = 676.04
Monoclinic, $P2_1/c$
a = 12.6481 (9) Å
b = 11.6659 (6) Å
c = 10.4922 (7) Å
β = 105.891 (7)°
V = 1488.98 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 293 K
0.03 × 0.03 × 0.02 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.983
4938 measured reflections
2626 independent reflections
1724 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.109
S = 1.02
2626 reflections
214 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N6^{i}	0.82	2.03	2.842 (4)	174
O1—H1B···N4^{ii}	0.85	2.07	2.868 (4)	157

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was supported by the Fundamental Research Funds for the Central Universities, P. R. China (No. SWJTU12CX048).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2206).

References

Braga, D., Polito, M., Giaffreda, S. L. & Grepioni, F. (2005). *Discuss. Faraday Soc.* pp. 2766–73.

Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (1997). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Faulmann, C., van Koningsbruggen, P. J., de Graaff, R. A. G., Haasnoot, J. G. & Reedijk, J. (1990). *Acta Cryst.* C**46**, 2357–2360.

Han, Z. B., Cheng, X. N. & Chen, X. M. (2005). *Cryst. Growth Des.* E**65**, 695–700.

Lin, J. B., Lin, R. B., Cheng, X. N., Zhang, J. P. & Chen, X. M. (2010). *Chem. Commun.* **47**, 9185–9187.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Xue, D. X., Lin, J. B., Zhang, J. P. & Chen, X. M. (2009). *CrystEngComm*, **11**, 183–188.

supplementary materials

Acta Cryst. (2012). E**68**, m1182–m1183 [doi:10.1107/S1600536812035428]

Diaquabis{3-[4-(1*H*-imidazol-1-yl)phenyl]-5-(pyridin-2-yl-κN)-1*H*-1,2,4-triazol-1-ido-κN^1}zinc

You-Song Wang, Guang-Mei Qiu and Cui-Juan Wang

Comment

The rational design and syntheses of metal-organic frameworks have been of increasing interest in the crystal engineering of coordination polymers owing to their ability to provide diverse assemblies with fascinating topological structures and material properties (Han *et al.*, 2005; Xue *et al.*,2009). The centrosymmetric unit of the title compound contains one Zn^{2+}ion, two Ippyt ligands and two coordination water molecules. For a similar structure, see: Braga *et al.* (2005); Lin *et al.* (2010); Faulmann *et al.* (1990). Every Zn^{II} ion is six-coordinated in a distorted octahedral coordination geometry by four N atoms from two Ippyt ligands and by two O atoms from two coordination water molecules (Fig. 1). There are two kinds of hydrogen bonding interactions which are between the coordinated waters and the triazolyl nitrogen atoms, and between the coordinated waters and the imidazolyl nitrogen atoms, respectively. However, the construct units are connected by the hydrogen bonding interactions between oxygen/ imidazolyl nitrogen atoms and imidazolyl nitrogen/ oxygen atoms from adjacent units respectively. Thus, infinite one-dimensional ring-shaped chains are formed. And then N3 and N3′ are further involved in forming another hydrogen bonding interactions with other neighbouring water oxygen atoms and thus connect the 1D supramolecular chains together to form the two-dimensional supramolecular architecture in the a,c plane. And finally the structures are interlinked alternately by different hydrogen bonding interactions and finally result in the three-dimensional supramolecular network architectures.(Fig.2).

Experimental

A mixture of $Zn(NO_3)_2.6H_2O$ (0.02 mmol), Ippyt (0.02 mmol), H2O (8 ml) was sealed in 25ml Teflon-lined stainless steel reactor, which was heated to 413 K for 5d and was subsequently cooled slowly to room temperature. Colourless block-shaped crystals were collected in 47% yield based on Zn.

Refinement

All H atoms were positioned geometrically (C-H = 0.93Åand O-H = 0.82 Å) and allowed to ride on their parent atoms, with U_{iso}(H) values equal to $1.2U_{eq}$(C) or $1.5U_{eq}$(O).

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

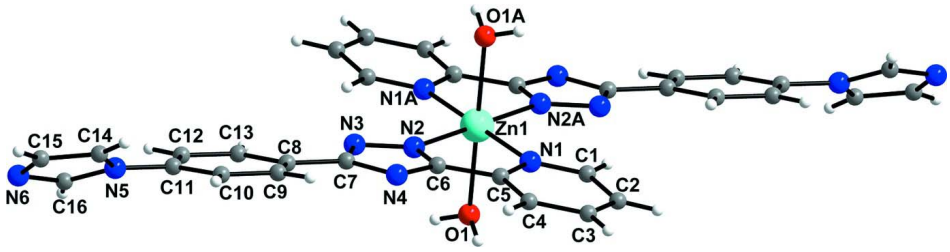


Figure 1

The coordination environment of Zn^{II} atom in the title compound.

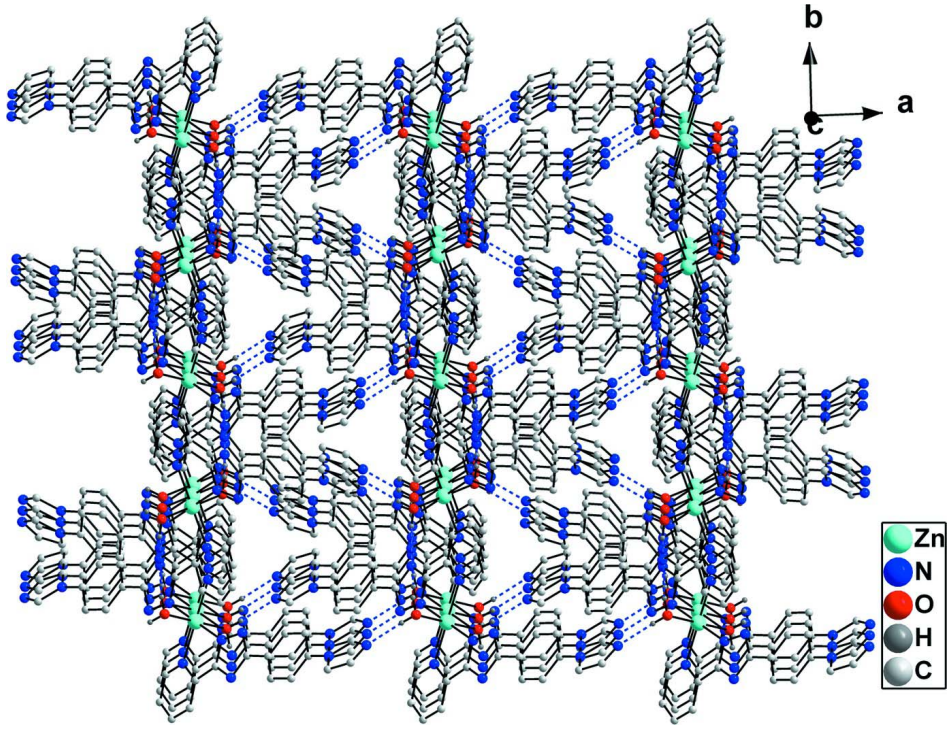


Figure 2

The 3D supermolecule network of the title compound. Dashed lines denote hydrogen bonds.

Diaquabis{3-[4-(1*H*-imidazol-1-yl)phenyl]-5-(pyridin-2-yl- κN)-1*H*-1,2,4-triazol-1-ido-κN^1}zinc

Crystal data

$[Zn(C_{16}H_{11}N_6)_2(H_2O)_2]$
$M_r = 676.04$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.6481\ (9)$ Å
$b = 11.6659\ (6)$ Å
$c = 10.4922\ (7)$ Å
$\beta = 105.891\ (7)°$
$V = 1488.98\ (16)$ Å^3
$Z = 2$
$F(000) = 700$
$D_x = 1.512$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1141 reflections
$\theta = 2.4–28.3°$
$\mu = 0.88$ mm^{-1}
$T = 293$ K
Block, colourless
0.03 × 0.03 × 0.02 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.983
4938 measured reflections
2626 independent reflections
1724 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −15→8
k = −12→13
l = −8→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.109
S = 1.02
2626 reflections
214 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.5000	0.0451 (2)
N1	0.4454 (2)	0.1728 (2)	0.4816 (3)	0.0390 (8)
N2	0.6022 (2)	0.0728 (2)	0.6718 (3)	0.0391 (8)
N3	0.6852 (2)	0.0414 (3)	0.7797 (3)	0.0441 (8)
N4	0.6357 (2)	0.2248 (2)	0.8079 (3)	0.0385 (8)
N5	1.0281 (2)	0.1265 (3)	1.3567 (3)	0.0553 (9)
N6	1.1782 (3)	0.0806 (3)	1.5144 (4)	0.0726 (12)
O1	0.62155 (17)	0.04131 (19)	0.3861 (3)	0.0481 (7)
H1B	0.6317	0.1134	0.3870	0.058*
H1	0.6799	0.0087	0.4200	0.072*
C1	0.3757 (3)	0.2195 (3)	0.3764 (4)	0.0469 (10)
H1A	0.3432	0.1729	0.3045	0.056*
C2	0.3496 (3)	0.3348 (3)	0.3698 (4)	0.0516 (11)
H2	0.3024	0.3661	0.2938	0.062*
C3	0.3952 (3)	0.4012 (3)	0.4776 (4)	0.0545 (11)
H3	0.3769	0.4784	0.4767	0.065*
C4	0.4682 (3)	0.3549 (3)	0.5884 (4)	0.0474 (10)

H4	0.4994	0.4000	0.6623	0.057*
C5	0.4938 (2)	0.2399 (3)	0.5865 (4)	0.0344 (8)
C6	0.5757 (3)	0.1811 (3)	0.6919 (4)	0.0347 (8)
C7	0.7019 (3)	0.1340 (3)	0.8583 (4)	0.0378 (9)
C8	0.7859 (3)	0.1342 (3)	0.9879 (4)	0.0393 (9)
C9	0.7952 (3)	0.2227 (3)	1.0774 (4)	0.0468 (10)
H9	0.7472	0.2846	1.0566	0.056*
C10	0.8756 (3)	0.2204 (3)	1.1987 (4)	0.0510 (11)
H10	0.8815	0.2811	1.2578	0.061*
C11	0.9465 (3)	0.1283 (3)	1.2313 (4)	0.0464 (10)
C12	0.9361 (3)	0.0383 (4)	1.1451 (5)	0.0595 (12)
H12	0.9823	−0.0249	1.1676	0.071*
C13	0.8562 (3)	0.0414 (3)	1.0237 (4)	0.0559 (11)
H13	0.8500	−0.0199	0.9655	0.067*
C14	1.0221 (4)	0.1771 (6)	1.4698 (5)	0.113 (2)
H14	0.9652	0.2232	1.4806	0.136*
C15	1.1136 (4)	0.1485 (5)	1.5641 (5)	0.114 (2)
H15	1.1299	0.1725	1.6519	0.137*
C16	1.1249 (3)	0.0693 (4)	1.3884 (5)	0.0675 (13)
H16	1.1507	0.0269	1.3280	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0514 (4)	0.0329 (3)	0.0373 (4)	0.0044 (3)	−0.0112 (3)	−0.0042 (4)
N1	0.0353 (16)	0.0368 (18)	0.037 (2)	0.0012 (14)	−0.0030 (14)	0.0003 (16)
N2	0.0400 (17)	0.0332 (17)	0.0352 (19)	0.0010 (13)	−0.0049 (14)	−0.0039 (15)
N3	0.0469 (18)	0.0380 (18)	0.036 (2)	0.0023 (14)	−0.0069 (15)	−0.0009 (17)
N4	0.0367 (16)	0.0354 (17)	0.0371 (19)	0.0015 (13)	−0.0005 (14)	−0.0029 (16)
N5	0.0367 (18)	0.082 (2)	0.040 (2)	0.0157 (17)	−0.0026 (15)	−0.002 (2)
N6	0.049 (2)	0.097 (3)	0.056 (3)	0.018 (2)	−0.0124 (19)	0.001 (3)
O1	0.0452 (14)	0.0400 (14)	0.0496 (18)	0.0068 (11)	−0.0032 (12)	0.0066 (14)
C1	0.048 (2)	0.048 (3)	0.033 (2)	0.0015 (18)	−0.0066 (18)	−0.001 (2)
C2	0.052 (2)	0.045 (2)	0.045 (3)	0.0087 (19)	−0.008 (2)	0.005 (2)
C3	0.059 (3)	0.038 (2)	0.056 (3)	0.0133 (19)	−0.002 (2)	0.000 (2)
C4	0.052 (2)	0.037 (2)	0.043 (3)	0.0054 (18)	−0.0035 (19)	−0.008 (2)
C5	0.0328 (19)	0.034 (2)	0.033 (2)	0.0002 (15)	0.0020 (16)	0.0004 (19)
C6	0.038 (2)	0.033 (2)	0.032 (2)	−0.0027 (16)	0.0065 (16)	−0.0031 (18)
C7	0.035 (2)	0.040 (2)	0.034 (2)	−0.0052 (16)	0.0028 (16)	−0.001 (2)
C8	0.034 (2)	0.042 (2)	0.036 (2)	0.0027 (16)	0.0006 (17)	0.002 (2)
C9	0.044 (2)	0.050 (2)	0.041 (3)	0.0092 (18)	0.0016 (18)	−0.003 (2)
C10	0.047 (2)	0.060 (3)	0.039 (2)	0.008 (2)	−0.0003 (19)	−0.015 (2)
C11	0.040 (2)	0.057 (3)	0.035 (2)	0.0064 (19)	−0.0021 (17)	0.001 (2)
C12	0.053 (3)	0.057 (3)	0.055 (3)	0.020 (2)	−0.007 (2)	−0.003 (3)
C13	0.056 (2)	0.050 (2)	0.051 (3)	0.009 (2)	−0.003 (2)	−0.010 (2)
C14	0.078 (4)	0.202 (7)	0.045 (3)	0.071 (4)	−0.008 (3)	−0.024 (4)
C15	0.074 (4)	0.209 (7)	0.041 (3)	0.057 (4)	−0.015 (3)	−0.018 (4)
C16	0.054 (3)	0.075 (3)	0.059 (3)	0.017 (2)	−0.009 (2)	−0.005 (3)

Geometric parameters (Å, º)

Zn1—N2^{i}	2.090 (3)	C2—C3	1.362 (5)
Zn1—N2	2.090 (3)	C2—H2	0.9300
Zn1—N1	2.123 (3)	C3—C4	1.381 (5)
Zn1—N1^{i}	2.123 (3)	C3—H3	0.9300
Zn1—O1^{i}	2.243 (2)	C4—C5	1.381 (4)
Zn1—O1	2.243 (2)	C4—H4	0.9300
N1—C1	1.326 (4)	C5—C6	1.463 (5)
N1—C5	1.353 (4)	C7—C8	1.479 (5)
N2—C6	1.339 (4)	C8—C9	1.378 (5)
N2—N3	1.366 (4)	C8—C13	1.385 (5)
N3—C7	1.340 (4)	C9—C10	1.396 (5)
N4—C6	1.346 (4)	C9—H9	0.9300
N4—C7	1.365 (4)	C10—C11	1.381 (5)
N5—C14	1.345 (6)	C10—H10	0.9300
N5—C16	1.353 (5)	C11—C12	1.368 (5)
N5—C11	1.433 (5)	C12—C13	1.393 (5)
N6—C16	1.316 (6)	C12—H12	0.9300
N6—C15	1.343 (6)	C13—H13	0.9300
O1—H1B	0.8500	C14—C15	1.342 (6)
O1—H1	0.8199	C14—H14	0.9300
C1—C2	1.382 (5)	C15—H15	0.9300
C1—H1A	0.9300	C16—H16	0.9300
N2^{i}—Zn1—N2	180.0	C3—C4—C5	118.2 (4)
N2^{i}—Zn1—N1	101.45 (11)	C3—C4—H4	120.9
N2—Zn1—N1	78.55 (11)	C5—C4—H4	120.9
N2^{i}—Zn1—N1^{i}	78.55 (11)	N1—C5—C4	121.2 (3)
N2—Zn1—N1^{i}	101.45 (11)	N1—C5—C6	114.4 (3)
N1—Zn1—N1^{i}	180.0	C4—C5—C6	124.4 (3)
N2^{i}—Zn1—O1^{i}	91.13 (10)	N2—C6—N4	113.4 (3)
N2—Zn1—O1^{i}	88.87 (10)	N2—C6—C5	118.7 (3)
N1—Zn1—O1^{i}	89.95 (10)	N4—C6—C5	127.8 (3)
N1^{i}—Zn1—O1^{i}	90.05 (10)	N3—C7—N4	114.3 (3)
N2^{i}—Zn1—O1	88.87 (10)	N3—C7—C8	121.3 (3)
N2—Zn1—O1	91.13 (10)	N4—C7—C8	124.5 (3)
N1—Zn1—O1	90.05 (10)	C9—C8—C13	118.2 (3)
N1^{i}—Zn1—O1	89.95 (10)	C9—C8—C7	122.2 (3)
O1^{i}—Zn1—O1	180.0	C13—C8—C7	119.6 (4)
C1—N1—C5	119.3 (3)	C8—C9—C10	120.8 (3)
C1—N1—Zn1	126.3 (3)	C8—C9—H9	119.6
C5—N1—Zn1	114.3 (2)	C10—C9—H9	119.6
C6—N2—N3	107.0 (3)	C11—C10—C9	120.1 (4)
C6—N2—Zn1	113.4 (2)	C11—C10—H10	119.9
N3—N2—Zn1	139.4 (2)	C9—C10—H10	119.9
C7—N3—N2	104.4 (3)	C12—C11—C10	119.7 (4)
C6—N4—C7	101.0 (3)	C12—C11—N5	120.7 (3)
C14—N5—C16	105.4 (4)	C10—C11—N5	119.6 (4)
C14—N5—C11	127.1 (3)	C11—C12—C13	119.9 (4)

C16—N5—C11	127.4 (4)	C11—C12—H12	120.0
C16—N6—C15	104.5 (4)	C13—C12—H12	120.0
Zn1—O1—H1B	109.3	C8—C13—C12	121.3 (4)
Zn1—O1—H1	109.7	C8—C13—H13	119.4
H1B—O1—H1	109.8	C12—C13—H13	119.4
N1—C1—C2	122.5 (4)	C15—C14—N5	107.2 (4)
N1—C1—H1A	118.8	C15—C14—H14	126.4
C2—C1—H1A	118.8	N5—C14—H14	126.4
C3—C2—C1	118.1 (4)	C14—C15—N6	110.7 (5)
C3—C2—H2	121.0	C14—C15—H15	124.6
C1—C2—H2	121.0	N6—C15—H15	124.6
C2—C3—C4	120.7 (3)	N6—C16—N5	112.2 (4)
C2—C3—H3	119.7	N6—C16—H16	123.9
C4—C3—H3	119.7	N5—C16—H16	123.9

Symmetry code: (i) $-x+1, -y, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N6^{ii}	0.82	2.03	2.842 (4)	174
O1—H1*B*···N4^{iii}	0.85	2.07	2.868 (4)	157

Symmetry codes: (ii) $-x+2, -y, -z+2$; (iii) $x, -y+1/2, z-1/2$.